THE PHASE EQUATION IN POTENTIAL SCATTERING

by

Terry Robert Dettmann

United States
Naval Postgraduate School

THESIS

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Terry Robert Dettmann
Lieutenant (junior grade), United States Navy
B.S., Marquette University, 1968

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ABSTRACT

The solutions of the phase equation for a potential with the asymptotic properties of an atomic polarization potential are studied with the intention of developing a computer program for direct integration of the phase equation for the s-wave phase shift of an arbitrary potential. Such a program is developed and its limitations are discussed. In addition, an appendix is devoted to the variational principles of Kohn and Schwinger for calculating phase shifts.

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LIST OF ILLUSTRATIONS

SYMBOLS

r	THE RADIAL COORDINATE IN BOHR RADII
K	THE ENERGY IN RYDBERGS
$\eta_o(r,K)$	THE PHASE-FUNCTION IN RADIANS
$\eta_o(K)$	THE PHASE SHIFT, $\eta_o(\infty,K)$, IN RADIANS
$u(r)$	THE SCHRODINGER RADIAL WAVE FUNCTION
$U(r)$ or $V(r)$	THE POTENTIAL FUNCTION IN RYDBERGS

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I. INTRODUCTION

The Quantum Theory of scattering processes is of basic importance in studies of atomic, nuclear, and elementary particle physics. Analysis of Atomic collision processes is required in such diverse applications as gas dynamics, chemical reaction theory, and stellar dynamics. Nuclear Physics relies on scattering of various particles from nuclei for a great deal of the quantitative information about nuclear processes while in Elementary Particle physics, very little other information is available except for the various scattering events that are observed.

There are many approaches to the scattering problem, but one of the most useful (especially in low energy applications) is the method of partial wave analysis. The method was first introduced by Faxen and Holtzmark based on a method developed by Lord Rayleigh. Rather then delve into the basis of the theory, it will be assumed that the reader is familiar with the treatment of Schiff [Ref. 1] or Merzbacher [Ref. 2].

A particularly interesting procedure for calculating scattering phase shifts is the "Phase Method." Originally introduced by Courant and Hilbert [Ref. 3] and applied to scattering by Morse and Allis [Ref. 4], the method has recently been revived and expanded in a series of papers by Calogero [Ref. 5, 6] and his new book [Ref. 7].

This paper will investigate the application of the phase equation to a potential which has the asymptotic properties of an atomic polarization potential ($1/r^4$). The method employed is a direct

integration of phase equation (11). In the appendix, the variational principles of Kohn and Schwinger are treated and are suggested as alternate methods for computation of phase shifts.

II. THEORY

A. THE PHASE FUNCTION METHOD

The phase function method is a method of reducing the second order linear Schrodinger Equation to a first order, non-linear Riccati equation. For s-wave scattering, the solution for phase shifts reduces to the solution of the differential equation

(1) $$\eta'(r) = -\left[V(r)/k\right]\sin^2(kr+\eta)$$

To show how this equation comes about, it is convenient to approach the problem from the standpoint of A. Ronveaux [Ref. 8]. He starts by considering a second-order homogeneous differential equation with two perturbative terms, $V_1(X)$ and $V_2(X)$;

(2) $$u'' + P(x)\,u' + Q(x)\,u = V_1(x)\,u + V_2(x)\,u'$$

with $u(0) = \mu$ and $u'(0) = \nu$. This can be written in the form of the following system

(3) $$X'(x) = A(x)\,X(x) + V(x)\,X(x)$$

where

$$X(x) = \begin{pmatrix} u \\ u' \end{pmatrix} \qquad X(0) = \begin{pmatrix} \mu \\ \nu \end{pmatrix}$$

$$A(X) = \begin{pmatrix} 0 & 1 \\ -Q & -P \end{pmatrix} \qquad V(X) = \begin{pmatrix} 0 & 0 \\ V_1 & V_2 \end{pmatrix}$$

The unperturbed solution, X_o is,

(4) $$X_o(x) = W(x)\,C$$

where $C = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$

is a constant vector, and

$$W(x) = \begin{pmatrix} u_1 & u_2 \\ u_1' & u_2' \end{pmatrix}$$

and u_1 and u_2 are two linearly independent solutions. The solution of the complete system may then be written

(5) $$Y(x) = W(x)\, C(x)$$

Using the Lagrange Method of Variation of Constants, then

$$C'(x) = \left\{ W(x) \right\}^{-1} V(x)\, W(x)\, C(x)$$

or

$$C'(x) = M(x) C(x)$$

where

$$C(0) = \left\{ W(0) \right\}^{-1} \begin{pmatrix} \mu \\ \nu \end{pmatrix}$$

If we now define the phase function

(6) $$S(x) = C_2(x) / C_1(x)$$

and differentiate, we find that

(7) $$S'(x) = M_{21}(x) + \left[M_{22}(x) - M_{11}(x) \right] S(x) - M_{12}(x) S^2(x)$$

Evaluating M gives the phase equation

(8) $$S'(x) = \left\{ \left[u_1(x) \right] + \left[u_2(x)\, S(x) \right] \right\} / \det W(x)$$
$$\times \left\{ V_1(x) \left[u_1(x) + u_2(x)\, S(x) \right] + V_2(x) \left[u_1'(x) + u_2'(x) S(x) \right] \right\}$$

where $\det(W) \neq 0$ and

$$S(0) = \frac{\left\{ \left[-u_1'(0) \mu \right] + \left[u_1(0) \nu \right] \right\}}{\left\{ \left[u_2'(0) \mu \right] + \left[u_2(0) \nu \right] \right\}}$$

Given the general form one now approaches the problem of s-wave phase shifts. The Schrodinger Equation (in natural units, $\hbar = c = 1$) is

$$u''(r) + k^2 u(r) = V(r)\, u(r) \tag{9}$$

choose

$$u(0) = \mu = 0$$

$$u'(0) = \nu$$

Then the general solution is

$$u(r) = c_1 \sin kr - c_2 \cos kr$$
$$= c_1(r)\left[\sin kr - S(r)\cos kr\right]$$

or

$$u(r) = c_1(r)\cos\eta_0(r,k)\sin(kr+\eta_0)$$

where

$$S(r) = c_2(r)/c_1(r) \equiv -\tan\eta_0(r,k)$$

Then, letting $V_1 = V$, $V_2 = 0$, $u_1 = \sin kr$, $u_2 = \cos kr$, $\det W = k$ the general phase equation becomes

$$(d/dr)\tan\eta_0 = -\left[V(r)/k\right]\left(\sin kr + \tan\eta_0 \cos kr\right)^2 \tag{10}$$

with $\tan\eta_0(0,k) = 0$. Noting that $(d/dr)\tan\eta_0 = \sec^2\eta_0 (d\eta_0/dr)$ it becomes apparent that

$$(d/dr)\eta_0 = -\left[V(r)/k\right]\sin^2(kr+\eta_0) \tag{11}$$

B. THE POTENTIAL FUNCTION

The object of this paper is to investigate the properties of the numerical solutions for the Phase Equation (11) when applied to a potential which has the asymptotic properties at infinity of an Atomic Polarization potential, i.e.,

$$U(r) \xrightarrow[r \to \infty]{} (\text{const.}) \times 1/r^4$$

In order to simplify the analysis, an additional condition was imposed on the potential in the form of a requirement that as $r \to 0$, the potential should approach zero as r, i.e.,

$$U(r) \xrightarrow[r \to 0]{} (\text{const.}) \times r$$

The function chosen to satisfy these conditions was

$$\mathcal{U}(r) = \frac{1}{r^4} \int_0^r dt\, t^4 e^{-t} \xrightarrow[r \to \infty]{} \frac{4!}{r^4}$$

The asymptotic properties of this form are obvious, however, it is difficult to calculate with. In order to simplify the problem further, the substitution $t = xr$ was chosen which leaves

$$U(r) = r \int_0^1 dx\, x^4 e^{-rx} \tag{12}$$

It is no longer readily apparent that U(r) has the correct asymptotic properties, but it may be easily verified by integration and power series expansion. The success of this form is shown in Fig. 1.

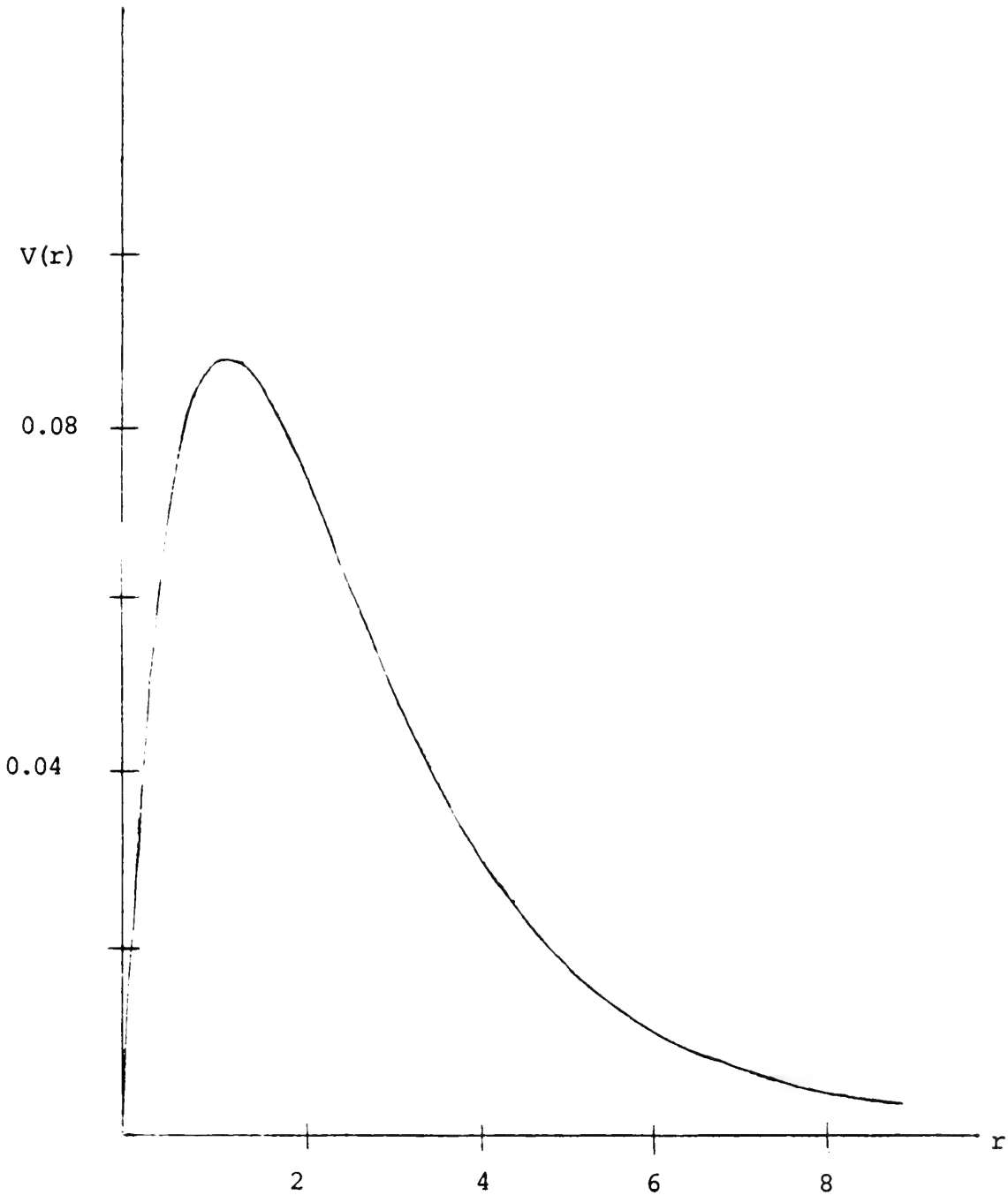

Figure 1

Plot of the Potential Function

III. CALCULATIONS

Having derived the phase equation (11), one now wishes to devise a method to put it to practical use. Calogero develops a variational scheme for the phase equation [Ref. 9] while other authors deal with the equation in other ways [Ref. 10, 11]. An excellent review has been prepared by Babikov [Ref. 12] which provides a good general introduction to actual calculations and an equally good bibliography. Owing to the fact that the equation is non-linear, the various approaches have dealt with some form of approximate solution. This paper will deal with the relatively simple problem of constructing a program to directly integrate the phase equation using numerical approximation only.

The particular method chosen was a fourth order Runge-Kutta Integration scheme to be implemented on the IBM-360 time sharing system. General discussions of the numerical method may be found in numerous places [Ref. 13, 14], and so only the necessary portion of that theory is presented here.

The Runge-Kutta method proposes to solve the equation

(13) $$y' = f(x, y)$$

subject to the initial conditions $X = X_o$ when $Y = Y_o$. The iterative solution process proceeds via the following equation;

(14) $$y_{n+1} = y_n + \frac{1}{6}\left[K_1 + 2K_2 + 2K_3 + K_4 \right]$$

where

$$K_1 = h f(x_n, y_n)$$

$$K_2 = h f\left(x_n + \tfrac{1}{2}h,\ y_n + \tfrac{1}{2}K_1\right)$$

$$K_3 = h f\left(x_n + \tfrac{1}{2}h,\ y_n + \tfrac{1}{2}K_2\right)$$

$$K_4 = h f(x_n + h, y_n + K_3)$$

and where $x_{n+1} = x_n + h$. The programming needed to provide a solution of the equation (11) which gives the exact phase shift, $\eta_0(K) = \eta_0(\infty, K)$, then reduces to programming a simple iterative procedure. The program developed is printed at the back and is in such a form that it may be run either on the time-sharing system for quick approximations or directly on the computer system in the regular batch processing. A second version of the program used to obtain a print out of the values of the phase function at various r values is also included. The use of the second form will become obvious as the discussion unfolds.

It now becomes necessary to consider the actual running of the program and its particular limitations. In order to properly investigate the program, the Yukawa potential,

$$V(r) = g e^{-mr}/mr$$

is convenient to consider since Calogero treats the case with strength parameter, g = -10, m = 1. The output produced by the second program is graphed in Figs. 2 and 3.

The most obvious feature of the graphs is the presence of "levels" which arise from the presence of possible bound states in the potential. Calogero discusses the connection of this with Levinson's theorem and shows that this structure in the phase function can be used to locate bound states. This very feature though poses a distinct problem to the evaluation of the exact phase shift. Owing to the presence of this structure, a simple test for the end of the integration that depends on the phase function tending to a constant value at infinity is useless.

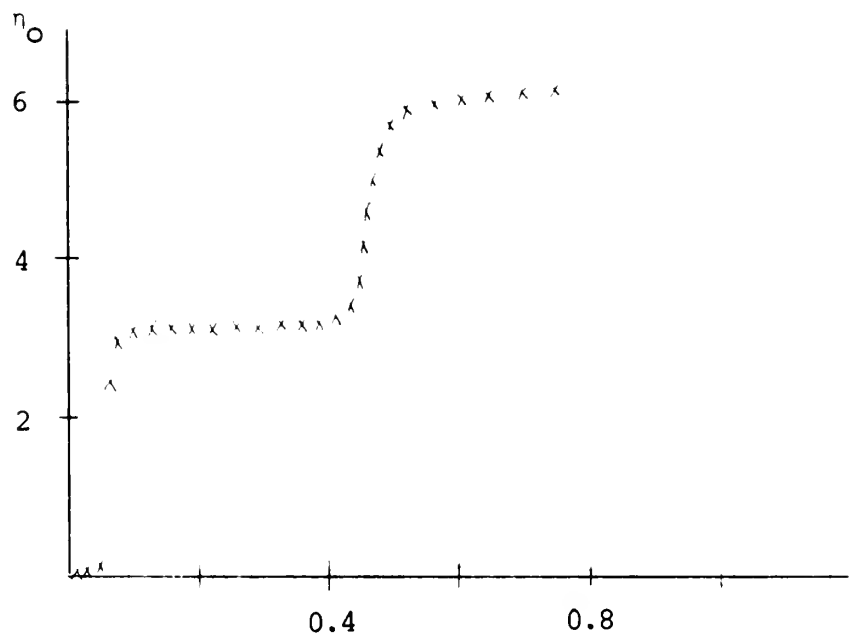

Figure 2

Plot of Phase Function for K = 0.1, Yukawa Potential

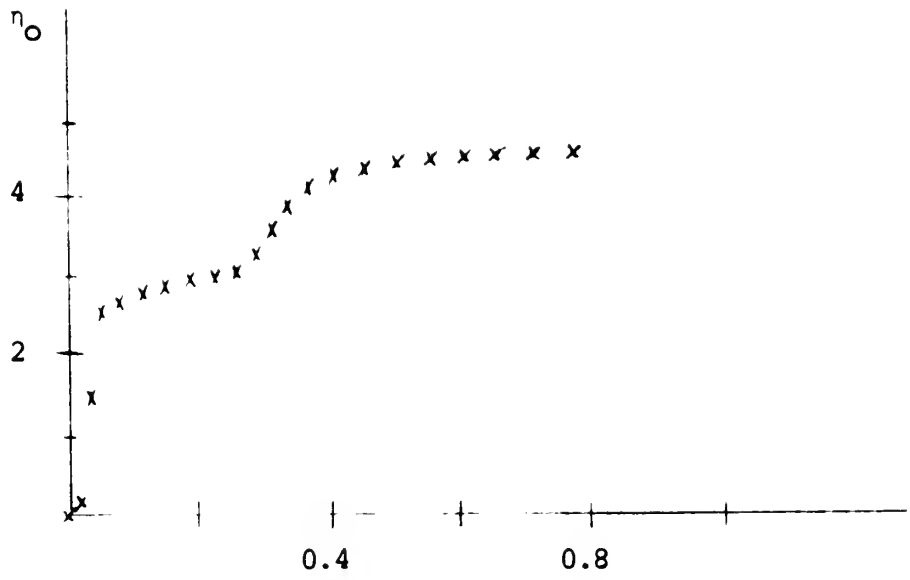

Figure 3

Plot of Phase Function for K = 1.0, Yukawa Potential

For this reason, the integration must be carried out past any possible structure before a cutoff of the above type is allowed. In order that the program will do just that, an integer counter is established and required to be larger than a certain lower limit which is designed to carry the integration over the structure. The procedure for doing this is as follows; the second form of the program is first run with the intention of finding the structure and determining the value of DR which gives the best results. Having found the structure, the counter may be set appropriately. By use of this artifice, the program is enabled to reproduce the results given in Calogero's book to within a few percent. It should be noted that another way of treating this problem is to establish a lower limit on the basis of the value of r reached. This approach would be superior if there were a method for predicting the position of the last flat region in η_o. The counter method was chosen only on the basis of a desire to know the number of iterations used, for computer timing purposes.

A further pecularity with the direct integration routine is the sensitivity to the x increment, DR. In investigations with different values of DR, it was found that when DR is chosen too large the structure at small r tends to destroy the accuracy of the routine by adding large terms over some of the flat regions in the phase function. An example is for K = 0.1 and dr = 0.1. The result is η_o = 44.1 in 110 steps as shown in the diagram (Fig. 4).

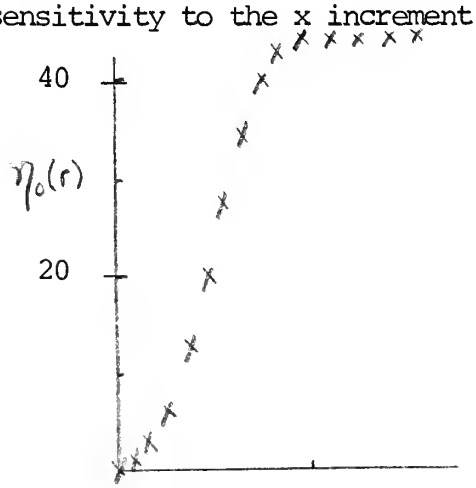

Figure 4

The true result (in agreement with Calogero's book, p. 22) is $\eta_o = 6.24$ in 38 steps found by taking dr = 0.01 or less. Now the utility of the second program for preliminary tests become apparent since it allows us to establish the number of bound states for the potential and the proper increment and the lower counter limit in just a few test runs which may be quickly run on the computer time sharing system.

The program also has a very important limitation in that the accuracy decreases sharply for a small k due to numerical round off errors arising from the necessity of dividing by a small number. The situation may be improved by choosing a smaller increment, DR, but after a certain point this procedure tends to become self defeating because decreasing DR increases the program running time. A test run on a Yukawa potential with g = -2, K = 0.1, and dr = 0.1 gives a close answer to the zero energy phase shift, but if the value of k is reduced to $K = 10^{-3}$, the accuracy in the calculated value of the phase shift actually decreases.

IV. RESULTS

The final problem is the application of the programs to the polarization potential discussed earlier, eqn. (12). Figures 5 and 6 detail the results of the explicit calculation with the second program. They indicate that a value of DR of 0.1 will carry the program nicely through to the asymptotic region if the lower counter limit is set at 200. The lack of structure in the graphs tends to make this requirement useless though and it becomes possible to set the limit at 10 iterations just to let the program get started before the asymptotic cutoff procedure is allowed to function. The lack of structure just commented on tends to indicate a lack of bound states in the potential as might be suspected from the very weak nature of the function. Tests could be done by imposing a strength parameter on the potential, i.e.,

$$V(r) = q\, r \int_0^1 dx\, x^d e^{-rx}$$

which could then be adjusted as suited the investigator. By means of such an artifice, bound states might begin to appear when the peak of the potential is high enough. In addition, increasing the strength of the potential would increase the magnitude of the phase shift. One might expect that such structure would appear for values of r less than 1.0 and that the way to locate such structure would be to decrease the value of the increment DR. Though interesting, such an investigation does not have any apparent physical use since the only physical feature of the potential is the asymptotic dependence at large r. Thus further discussion of this point has been omitted here.

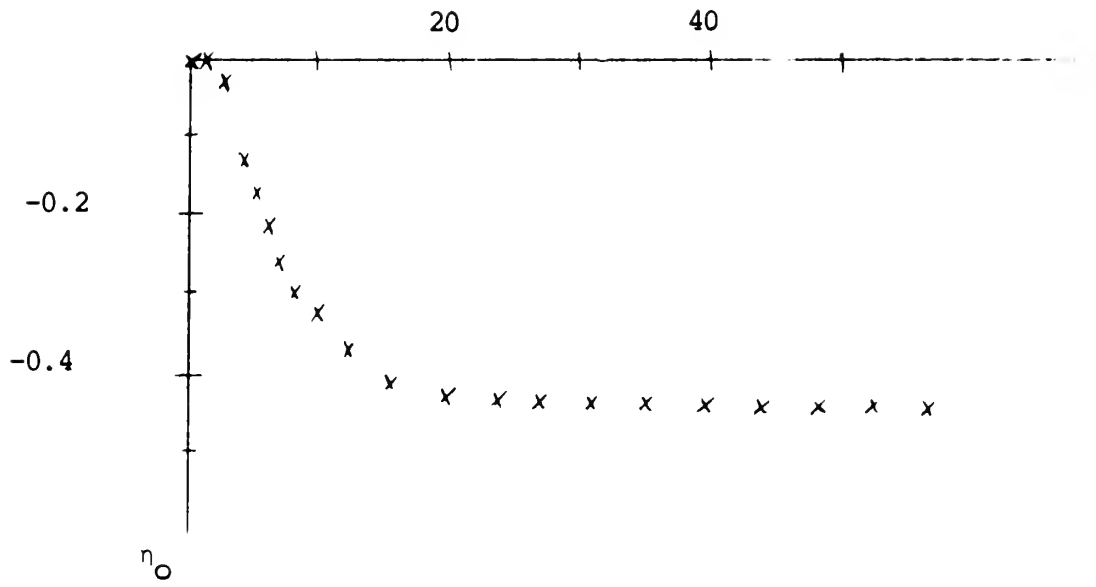

Figure 5

Plot of Phase Function for K = 0.1, Polarization Potential

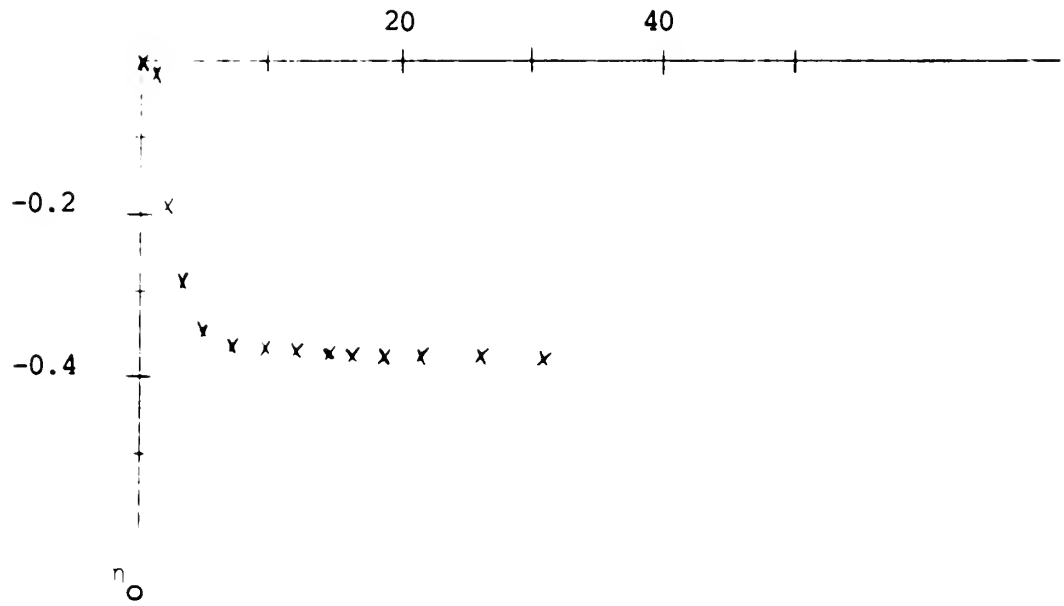

Figure 6

Plot of Phase Function for K = 1.0, Polarization Potential

The most interesting feature of the calculation from the standpoint of possible application of the program to real, physical potentials is the necessity of carrying out the calculation to larger values of the radial coordinate than was the case for the Yukawa potential. The reason for this behavior is obvious, the polarization potential only drops off as fast as $1/r^4$ at infinity. This leads to the observed difference in the convergence of the scheme and probably to the reason why the only places that the Phase method is applied in the literature are in papers dealing with nuclear type potentials which may be assumed to fall off very rapidly. To get some idea of the magnitude of this effect, the graph in Fig. 2 may be examined in comparison to the graph in Fig. 5. The plot for the Yukawan potential has stabilized by r = 1 while with the polarization potential, the plot is just stabilizing at r = 25. These observations hold great import for any application of the method to atomic like potentials since the matter of time available for computation is often very critical. Even on the IBM-360 time sharing system, timing for the program had become critical when increments less than 0.1 were chosen. In addition, output disk space became a problem. The problem of timing could be expected to be considerable worse on smaller computing systems.

Having discussed the phase function and its properties, use may now be made of program 1 to obtain a plot of η_o vs. energy as in Fig. 7. The most apparent feature of Fig. 7 is the 0.78 radian peak at k = 0.36. It is a real peak as opposed to an apparent peak that could be produced by a poor choice of the increment at such a low value of k. An interpretation of this peak will not be attempted at this point but a comment is appropriate on the behavior of $\eta_o(K)$ on the low energy portion

of the peak. It seems to drop off drastically, possibly to zero. Below k = 0.1, no data taking was attempted due the necessity of integrating too far with too small an increment.

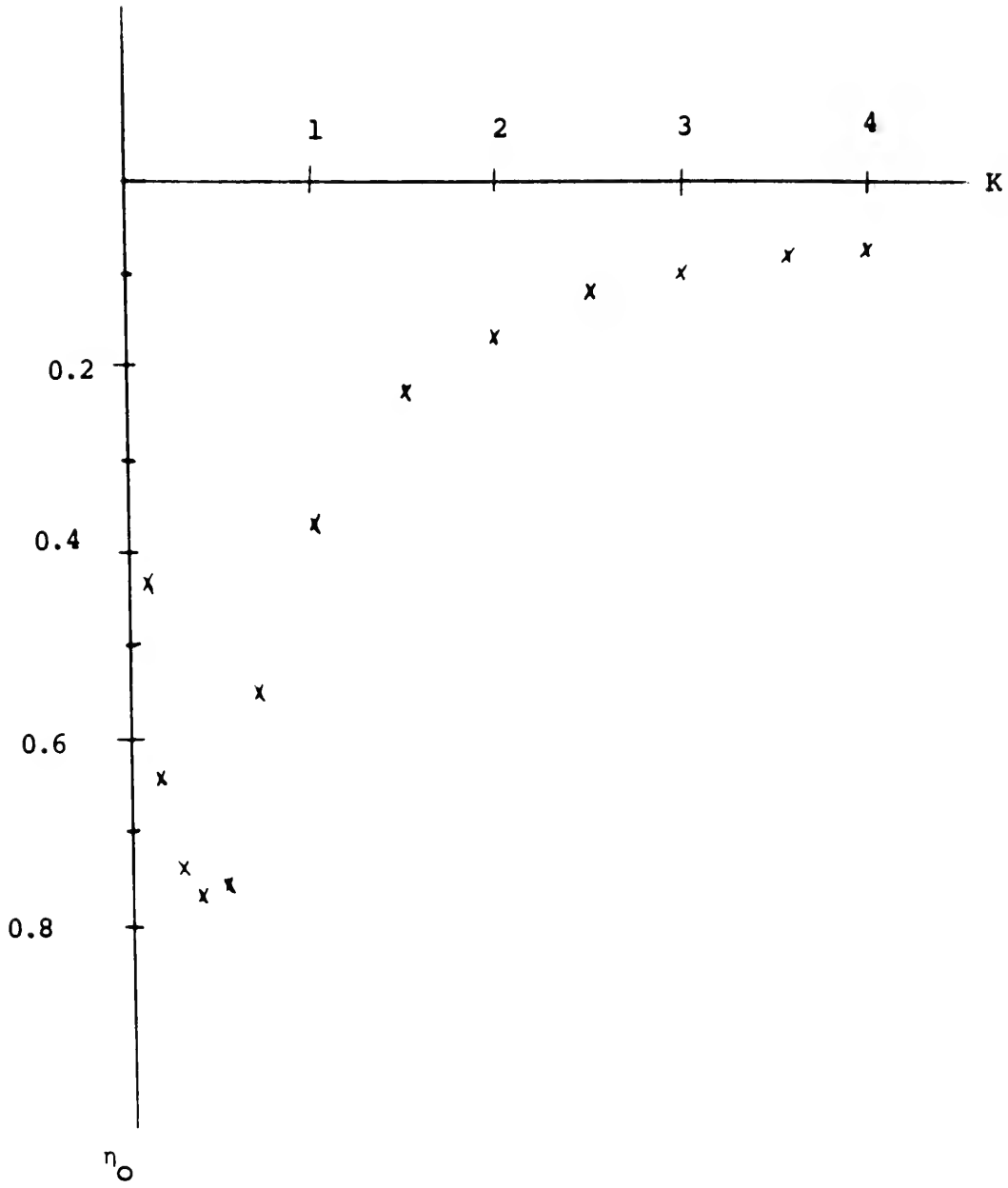

Figure 7

Plot of Phase Shift vs. K for Polarization Potential

V. CONCLUSIONS

The program developed for the phase equation integration has been tried on a test case and applied to a second, semi-physical case with somewhat the expected results. This program has in these two cases performed well as long as the precautions mentioned were taken. It should be noted that no error analysis of the routine was attempted due to lack of time, however, the comparison of the results on the Yukawa potential for g = -10 with the results published by Calogero in his book [Ref. 7], tends to point to an accuracy that is within a few percent. Whether this result is valid for any potential other than the Yukawa potential and in particular whether it is equally true for atomic level potentials is a question that remains unanswered at this point. It is expected that simple numerical errors arising from the Runge-Kutta integration scheme and the ordinary computer errors of round off, etc. will decrease the accuracy of the calculation.

APPENDIX

(A.1) The Kohn-Hulthen Method

The most frequently used variational procedure is the Kohn-Hulthen method [Ref. 15, 16] which is based on the stationary property of the functional $\lambda + I$ where

$$I = \frac{2m}{\hbar^2} \int \psi (E - H) \psi \, d\tau \tag{A1}$$

and λ is some function of the phase shift determined from the normalization of ψ as $r \to \infty$. This paper will employ tangent normalization throughout, i.e.,

$$\psi \xrightarrow[r \to \infty]{} (4\pi)^{-\frac{1}{2}} \left[j_\ell(kr) + \tan\eta_\ell \, n_\ell(kr) \right] \tag{A2}$$

where η_ℓ is the phase shift for the ℓ^{th} partial wave and j_ℓ and n_ℓ are the spherical Bessel and Neuman functions respectively. Considering the special case of s-wave scattering, $\ell = 0$, then (A2) becomes

$$\psi \longrightarrow (4\pi)^{-\frac{1}{2}} \left[\sin kr/kr + \tan\eta_0 \cos kr/kr \right]$$
$$= (4\pi)^{-\frac{1}{2}} \frac{1}{\cos\eta_0} \frac{\sin(kr + \eta_0)}{kr}$$

With this form for ψ, one now considers the explicit variation of (A1)

$$\delta I = \int \delta\psi (\nabla^2 + k^2 - U) \psi \, d\tau + \int \psi (\nabla^2 + k^2 - U) \delta\psi \, d\tau \tag{A3}$$

Since for s-wave, ψ has no angular dependence,

$$\nabla^2 \psi = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) \psi$$

so that the second integral in (A3) becomes

$$\int \psi \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + k^2 - U \right] \delta\psi \, d\tau$$
$$= \int_0^{2\pi} d\Omega \int_0^{\pi} \sin\theta \, d\theta \int_0^{\infty} dr \, \psi \frac{d}{dr} \left[r^2 \frac{d(\delta\psi)}{dr} \right] + \int \delta\psi (k^2 - U) \psi \, d\tau$$

Integrating by parts, this gives

$$= 4\pi \int_0^\infty dr \left\{ \frac{d}{dr}\left[\psi r^2 \frac{d(\delta\psi)}{dr} \right] - \frac{d\psi}{dr} r^2 \frac{d}{dr}(\delta\psi) \right. \\ \left. + \int \delta\psi (K^2 - U)\psi \, d\tau \right.$$

$$= 4\pi \int_0^\infty dr \left\{ \frac{d}{dr}\left[\psi r^2 \frac{d}{dr}(\delta\psi) - \delta\psi r^2 \frac{d\psi}{dr} \right] + \delta\psi \frac{d}{dr}\left(r^2 \frac{d\psi}{dr} \right) \right. \\ \left. + \int \delta\psi (K^2 - U)\psi \, d\tau \right.$$

$$= 4\pi \int_0^\infty dr \frac{d}{dr}\left[\psi r^2 \frac{d(\delta\psi)}{dr} - \delta\psi r^2 \frac{d\psi}{dr} \right] + \frac{2m}{\hbar^2} \int \delta\psi (E - H)\psi \, d\tau$$

Thus (A3) becomes

$$\delta I = 2 \int \delta\psi (\nabla^2 + K^2 - U)\psi \, d\tau + 4\pi \left[r^2 \left(\psi \frac{d\delta\psi}{dr} - \delta\psi \frac{d\psi}{dr} \right) \right]_0^\infty$$

The last term, upon application of the boundary conditions, reduces to $-\delta(\tan\eta_0/K)$ so that

(A4) $$\delta(I + \tan\eta_0/K) = 2 \int \delta\psi (\nabla^2 + K^2 - U)\psi \, d\tau$$

But the Schrodinger equation is just

$$(\nabla^2 + K^2 - U)\psi = 0$$

so that

(A5) $$\delta(I + \tan\eta_0/K) = 0$$

The stationary functional, $[\lambda] = \tan\eta_0/K$, is given by

(A6) $$[\lambda] = \lambda + I = \lambda + \frac{2m}{\hbar^2} \int \psi (E - H)\psi \, d\tau$$

The trial function, ψ, is chosen to have the form

(A7) $$\psi = \varphi + \sum c_i \chi_i(r)$$

where $\varphi = (4\pi)^{-\frac{1}{2}}[j_0 - \lambda k j_1]$ and the χ_i are some convenient basis functions, that rapidly approach zero as $r \to \infty$. The asymptotic part of the wave function φ, is chosen so as to shield the $\frac{1}{r}$ singularity in cos kr/r as $r \to 0$. It is evident that φ has the correct asymptotic form as

$$\varphi = (4\pi)^{-\frac{1}{2}}\left[\sin kr/kr - \lambda k(\sin kr/k^2r^2 - \cos kr/kr)\right]$$

$$\xrightarrow[r \to \infty]{} (4\pi)^{-\frac{1}{2}}\left[(\sin kr/kr) + \lambda(\cos kr/r)\right]$$

The Kohn-Hulthen principle then states that the variation of $[\lambda]$ with respect to all arbitrary constants, i.e.,

(A8) $$\delta[\lambda] = \delta(\lambda + I) = 0$$

produces a value of $[\lambda]$ that is second order accurate in $\delta\lambda$. The explicit variation is done by writing the functional in the form;

(A9) $$[\lambda] = \sum_{ij} c_i c_j M_{ij} + 2\sum_j c_j R_j + B + \lambda$$

where

$$M_{ij} = \frac{2m}{\hbar^2}\int \chi_i(E - H)\chi_j = M_{ji}$$

$$R_j = \frac{2m}{\hbar^2}\int \chi_j(E - H)\varphi$$

$$B = \frac{2m}{\hbar^2}\int \varphi(E - H)\varphi$$

Variation of the n constants, C_i then gives the system of linear equations

(A10) $$\sum_j M_{ij} C_j = - R_i$$

Since the trial function is linear in λ,

$$R_i = R_i^{(0)} + \lambda R_i^{(1)}$$

and since the M_{ij} are independent of λ

$$C_i = C_i^{(0)} + \lambda C_i^{(1)}$$

This leaves the equations:

(A11) $$\sum_j M_{ij} C_j^{(0)} = - R_i^{(0)}$$
$$\sum_j M_{ij} C_j^{(1)} = - R_i^{(1)}$$

Solving for the constants,

$$[\lambda] = W_0 + \lambda W_1 + \lambda^2 W_2 + B_0 + \lambda B_1 + \lambda^2 B_2 + \lambda$$

where

$$W_0 = \sum_{ij} C_i^{(0)} M_{ij} C_j^{(0)} + 2 \sum_i C_i^{(0)} R_i^{(0)}$$

$$W_1 = \sum_{ij} C_i^{(0)} M_{ij} C_j^{(1)} + 2 \sum_i C_i^{(0)} R_i^{(1)} + 2 \sum_i C_i^{(1)} R_i^{(0)}$$

$$W_2 = \sum_{ij} C_i^{(1)} M_{ij} C_j^{(1)} + 2 \sum_i C_i^{(1)} R_i^{(1)}$$

Then a final variation with respect to λ gives, to first order

$$\lambda = - \frac{(W_1 + B_1 + 1)}{2(W_2 + B_2)}$$

and the second order accurate, stationary functional is

(A12) $$[\lambda] = W_0 + B_0 - \frac{(W_1 + B_1 + 1)^2}{4(W_2 + B_2)}$$

(A.2) The Schwinger Method

A less frequently used but more elegant variational method is that due to Schwinger [Ref. 17, 18, 19, 20]. It gives the stationary value of the functional $[K\cot\eta]$ directly. The problem is to solve the radial Schrodinger Equation.

$$\frac{d^2 u_\ell}{dr^2} + \left[K^2 - \frac{\ell(\ell+1)}{r^2} \right] u_\ell(r) = U(r)\, u_\ell(r) \tag{A13}$$

To do so, one solves for the Green's Function $G_\ell(r|r_0)$ given by,

$$\frac{d^2}{dr^2} G_\ell(r|r_0) + \left[K^2 - \frac{\ell(\ell+1)}{r^2} \right] G_\ell(r|r_0) = -\delta(r-r_0) \tag{A14}$$

which gives

$$\begin{aligned} G_\ell(r|r_0) &= -Krr_0\, j_\ell(Kr)\, n_\ell(Kr_0) \qquad r \le r_0 \\ &= -Krr_0\, j_\ell(Kr_0)\, n_\ell(Kr) \qquad r_0 \le r \end{aligned} \tag{A15}$$

The integral equation for $u_\ell(r)$ is then

$$u_\ell(r) = Kr\, j_\ell(Kr) - \int_0^\infty dr_0\, G_\ell(r|r_0)\, U(r_0)\, u_\ell(r_0) \tag{A16}$$

For large r, the asymptotic forms are

$$Kr\, j_\ell(Kr) \longrightarrow \cos\left(Kr - \tfrac{1}{2}(\ell+1)\pi\right)$$

$$Kr\, n_\ell(Kr) \longrightarrow \sin\left(Kr - \tfrac{1}{2}(\ell+1)\pi\right)$$

therefore, the asymptotic form of $u_\ell(r)$ may be written as

$$\begin{aligned} u_\ell(r) \longrightarrow\ & \cos\left[Kr - \tfrac{1}{2}(\ell+1)\pi\right] \\ & + \sin\left[Kr - \tfrac{1}{2}(\ell+1)\pi\right] \int_0^\infty dr_0\, r_0\, j_\ell(Kr_0)\, U(r_0)\, u(r_0) \end{aligned} \tag{A17}$$

But, this is to match to the asymptotic form

$$u_\ell(r) \longrightarrow \cos\left[Kr - \tfrac{1}{2}(\ell+1)\pi\right] + \sin\left[Kr - \tfrac{1}{2}(\ell+1)\pi\right] \tan\eta_\ell$$

and so one sets

$$\tan\eta_\ell = \int_0^\infty dr_0\, r_0\, j_\ell(kr_0)\; U(r_0)\, u_\ell(r_0)$$

Inserting the integral form for $j_\ell(kr)$ in terms of $u_\ell(r)$ from (A16)

$$\tan\eta_\ell = \frac{1}{K}\int_0^\infty dr\; U(r)\, u_\ell(r)\left[u_\ell(r) + \int_0^\infty G(r|r_0)\; U(r_0)\, u_\ell(r_0)\, dr_0\right]$$

therefore,

$$K\tan\eta_\ell = \int_0^\infty dr\; U(r)\, u_\ell^2(r) + \int_0^\infty dr \int_0^\infty dr_0\, U(r)\, u_\ell(r)\, G(r|r_0)\, U(r_0)\, u_\ell(r_0)$$

dividing now by $\tan^2\eta_\ell$

$$\text{(A18)}\quad K\cot\eta_\ell = \frac{\int_0^\infty dr\, U(r)\, u_\ell^2(r) + \int_0^\infty dr \int_0^\infty dr_0\, U(r)\, u_\ell(r)\, G_\ell(r|r_0)\, U(r_0)\, u_\ell(r_0)}{\left[\int_0^\infty dr\; r\; U(r)\, u_\ell(r)\, j_\ell(kr)\right]^2}$$

For s-waves this becomes

$$\text{(A19)}\quad K\cot\eta_0 = \frac{\int_0^\infty dr\; U(r)\, u^2(r) - \int_0^\infty dr \int_0^\infty dr_0\; U(r)\, u(r)\, G(r|r_0)\, U(r_0)\, u(r_0)}{\left[\frac{1}{K}\int_0^\infty dr\; U(r)\, u(r)\sin kr\right]^2}$$

where $G(r|r_0)$ is now:

$$G(r|r_0) = \frac{1}{K}\sin kr\cos kr_0 \qquad r \le r_0$$

$$= \frac{1}{K}\sin kr_0\cos kr \qquad r_0 \le r$$

In order to show that (A19) is in fact stationary to second order for the exact wave function, consider

$$\text{(A20)}\qquad \delta[K\cot\eta] = [K\cot\eta(u+\delta u)] - [K\cot\eta(u)]$$

Expanding and collecting terms, we have

$$\delta[k\cot\eta_0] = \frac{\int_0^\infty dr\, U(r)u(r)\left[u(r) - \int_0^\infty dr_0\, G(r|r_0)\,U(r_0)u(r_0)\right] + 2\int_0^\infty dr\, U(r)\delta u\left[u(r) - \int_0^\infty G(r|r_0)\,U(r_0)u(r_0)\right]}{\left[\frac{1}{k}\int_0^\infty dr\, U(r)u(r)\sin kr\right]^2 + 2\left[\frac{1}{k}\int_0^\infty dr\, U(r)\delta u\sin kr\right]\times\left[\frac{1}{k}\int_0^\infty dr\, U(r)u(r)\sin kr\right]}$$

$$- \frac{\int_0^\infty dr\, U(r)u(r)\left[u(r) - \int_0^\infty dr_0\, G(r|r_0)\,U(r_0)u(r_0)\right]}{\left[\frac{1}{k}\int_0^\infty dr\, U(r)u(r)\sin kr\right]^2} + O(\delta^2)$$

combining the terms the numerator for the expression will be

$$\left[\frac{1}{k}\int_0^\infty dr\, U(r)u(r)\sin kr\right]^2\left\{\int_0^\infty dr\, U(r)u(r)\left[u(r) - \int_0^\infty dr_0\, G(r|r_0)\,U(r_0)u(r_0)\right] + 2\int_0^\infty dr\, U(r)\delta u(r)\left[u(r) - \int_0^\infty dr_0\, G(r|r_0)\,U(r_0)u(r_0)\right]\right\}$$

$$- \int_0^\infty dr\, U(r)u(r)\left[u(r) - \int_0^\infty dr_0\, G(r|r_0)\,U(r_0)u(r_0)\right]\left\{\left[\frac{1}{k}\int_0^\infty dr\, U(r)u(r)\sin kr\right]^2 + 2\left[\frac{1}{k}\int_0^\infty dr\, U(r)\delta u(r)\sin kr\right]\times\left[\frac{1}{k}\int_0^\infty dr\, U(r)u(r)\sin kr\right]\right\} + O(\delta^2)$$

However

$$\text{(A21)}\qquad \int_0^\infty dr\, U(r)u(r)\left[u(r) - \int_0^\infty dr_0\, G(r|r_0)\,U(r_0)u(r_0)\right] = k\cot\eta_0\left[\frac{1}{k}\int_0^\infty dr\, U(r)u(r)\sin kr\right]^2$$

but from (A17) this is

$$= \int_0^\infty dr\, U(r)u(r)\sin kr$$

After factoring out $\left[\frac{1}{k}\int dr\, U(r)u(r)\sin kr\right]^2$, the numerator becomes

$$\left[\frac{1}{k}\int_0^\infty dr\, U(r)u(r)\sin kr\right]^2\left\{\int_0^\infty dr\, U(r)u(r)\sin kr - \int_0^\infty dr\, U(r)u(r)\sin kr + 2\int_0^\infty dr\, U(r)\delta u(r)\left[u(r) - \sin kr - \int_0^\infty dr_0\, G(r|r_0)\,U(r_0)u(r_0)\right]\right\} + O(\delta^2)$$

However, combining terms, this is,

$$\left[\frac{1}{K}\int_0^\infty dr\, U(r)u(r)\sin kr\right]^2\left\{2\int_0^\infty dr\, U(r)\delta u(r)\left[u(r)-\sin kr-\int_0^\infty dr_0\, G(r|r_0)\,U(r_0)u(r_0)\right]\right.$$
$$+\ \mathcal{O}(\delta^2)$$

But from (A16), for u(r) the correct wave function,

$$u(r)-\sin kr-\int_0^\infty dr_0\, G(r|r_0)\,U(r_0)u(r_0)\equiv 0$$

Thus, neglecting terms of order δ^2, the numerator is zero and hence

$$\delta[K\cot\eta_0]=0$$

Therefore, we see that (neglecting second order variations) the expression is stationary when u is the correct solution of the Schrodinger Equation.

Now going back to equation (A19) and inverting

$$(A24)\quad [K\tan\eta_0]=\frac{\left[\int_0^\infty dr\, U(r)u(r)\sin kr\right]^2}{\int_0^\infty dr\, U(r)u^2(r)-\int_0^\infty dr\int_0^\infty dr_0\, U(r)u(r)G(r|r_0)U(r_0)u(r_0)}$$

Letting $u(r)=\sum c_i\chi_i$ then

$$(A25)\quad [K\tan\eta_0]=\frac{\left(\sum c_i V_i\right)^2}{\sum c_i c_j\,(U_{ij}-G_{ij})}=\frac{\sum c_i c_j N_{ij}}{\sum c_i c_j M_{ij}}$$

where

$$V_i=\int_0^\infty dr\, U(r)\,\chi_i(r)\sin kr$$

$$U_{ij}=\int_0^\infty dr\, U(r)\,\chi_i(r)\,\chi_j(r)=U_{ji}$$

$$G_{ij}=\int_0^\infty dr\int_0^\infty dr_0\, U(r)\,\chi_i(r)G(r|r_0)U(r_0)\chi_j(r_0)=G_{ji}$$

and

$$N_{ij}=V_iV_j=N_{ji}\qquad M_{ij}=U_{ij}-G_{ij}$$

The problem remaining is to solve for $[K\tan\eta_0]$ and the C_s'. To do so, define

(A26) $$Q \equiv \sum c_i c_j \left([K\tan\eta_0] M_{ij} - N_{ij} \right) \equiv 0$$

but Q is obviously stationary and so,

(A27) $$\frac{\partial Q}{\partial c_i} = 2 \sum c_j \left([K\tan\eta_0] M_{ij} - N_{ij} \right) = 0$$

In order to have a solution for the C_s', the determinant of the matrix of coefficients must be zero, i.e.,

(A28) $$\det \left([K\tan\eta_0] M_{ij} - N_{ij} \right) = 0$$

However, it is a simple matter to show that the matrix N is of rank one, i.e., there are no non-zero sub-determinants of the matrix N of order 2, and further, it can be shown that such a system has only one nontrivial solution for $[K\tan\eta_0]$.

(A29) $$[K\tan\eta_0] = \frac{\begin{vmatrix} N_{11} & N_{12} & \cdots \\ M_{21} & M_{22} & \cdots \\ \vdots & & \end{vmatrix} + \begin{vmatrix} M_{11} & M_{12} & \cdots \\ N_{21} & N_{22} & \cdots \\ \vdots & & \end{vmatrix} + \cdots}{\begin{vmatrix} M_{ij} \end{vmatrix}}$$

Thus one finds the solution for $[K\tan\eta]$ without recourse to a solution for the C_s'. This result is shown in Kohn's Paper [Ref. 15].

```
C                                                                       PHF00001
C                                                                       PHF00002
C      THE PURPOSE OF THIS PROGRAM IS TO PERFORM                        PHF00003
C        A RUNGE-KUTTA INTEGRATION OF THE CALOGERO                      PHF00004
C        PHASE FUNCTION EQUATION TO OBTAIN THE                          PHF00005
C        SCATTERING PHASE SHIFT FOR AN ARBITRARY                        PHF00006
C        POTENTIAL P(R)                                                 PHF00007
CC                                                                      PHF00008
C                                                                       PHF00009
       EXTERNAL P                                                       PHF00010
       REAL K1,K2,K3,K4                                                 PHF00011
    4  CONTINUE                                                         PHF00012
C                                                                       PHF00013
C   READS IN VALUES OF ENERGY IN RYDBERGS AND INCREMENT IN ATOMIC UNITS PHF00014
C                                                                       PHF00015
       READ 100,E,DR                                                    PHF00016
       IF(E .EQ. 0.0) GO TO 3                                           PHF00017
       AETA = 0.0                                                       PHF00018
       ETA = 0.0                                                        PHF00019
       R = 0.0                                                          PHF00020
C                                                                       PHF00021
C   INITIALIZE THE INTEGER COUNTER K WHICH COUNTS THE                   PHF00021
C   NUMBER OF ITERATIONS AND HENCE THE NUMBER OF INCREMENTS             PHF00021
C   DR IN THE INTEGRATION                                              PHF00021
C                                                                       PHF00021
       K = 0                                                            PHF00021
    1  CONTINUE                                                         PHF00022
C                                                                       PHF00023
C   BEGINNING OF INTEGRATION LOOP                                       PHF00024
C                                                                       PHF00025
       AETA = ETA                                                       PHF00026
       K1 = DR*F(R,ETA,E,P)                                             PHF00027
       K2 = DR*F(R+0.5*DR,ETA+0.5*K1,E,P)                               PHF00028
       K3 = DR*F(R+0.5*DR,ETA+0.5*K2,E,P)                               PHF00029
       K4 = DR*F(R+DR,ETA+K3,E,P)                                       PHF00030
       ETA = ETA + (K1 + 2.*K2 + 2.*K3 + K4)/6.                         PHF00031
       R = R + DR                                                       PHF00032
       K = K + 1                                                        PHF00033
C                                                                       PHF00034
C   TESTS FOR EXIT FROM INTEGRATION LOOP                                PHF00035
C                                                                       PHF00036
       TEST = ABS((ETA-AETA)/ETA)                                       PHF00037
       IF(K .LT. 1000 ) GO TO 1                                         PHF00038
       IF( TEST .LT. 1.0E-08) GO TO 2                                   PHF00039
       IF( K .GT. 18000) GO TO 2                                        PHF00040
       GO TO 1                                                          PHF00041
    2  CONTINUE                                                         PHF00042
       TNE = TAN(ETA)/E                                                 PHF00043
```

```
      PRINT 103                                                          PHF00044
      PRINT 101,E,ETA,TNE                                                PHF00045
      PRINT 102,K,TEST                                                   PHF00046
      PRINT 103                                                          PHF00047
      GO TO 4                                                            PHF00048
    3 CONTINUE                                                           PHF00049
      STOP                                                               PHF00050
  100 FORMAT(2F10.0)                                                     PHF00051
  101 FORMAT(T2,'CALOGERO PHASE SHIFT'/T5,'K = ',T9,1PE10.3/             PHF00052
     1    T5,'ETA = ',T11,1PE15.8/T5,'TANGENT(ETA)/K = ',T22,1PE15.8)   PHF00053
  102 FORMAT(//2X4HK = ,I6/2X7HTEST = ,1PE10.3)                          PHF00054
  103 FORMAT(///)                                                        PHF00055
      END                                                                PHF00056



      FUNCTION F(R,ETA,E,P)                                              PHF00057
C                                                                        PHF00058
C   THIS FUNCTION PROVIDES THE MAINLINE INTEGRATION ROUTINE              PHF00059
C   WITH THE FUNCTION                                                    PHF00060
C                                                                        PHF00061
C         -P(R)*SIN(KR+ETA)**2                                           PHF00062
C                                                                        PHF00063
C                                                                        PHF00064
      EXTERNAL P                                                         PHF00065
      F = -P(R)*SIN(E*R+ETA)**2/E                                        PHF00066
      RETURN                                                             PHF00067
      END                                                                PHF00068
```

```
C                                                                       PHF00001
C                                                                       PHF00002
C       THE PURPOSE OF THIS PROGRAM IS TO PERFORM                       PHF00003
C         A RUNGE-KUTTA INTEGRATION OF THE CALOGERO                     PHF00004
C         PHASE FUNCTION EQUATION TO OBTAIN THE                         PHF00005
C         SCATTERING PHASE SHIFT FOR AN ARBITRARY                       PHF00006
C         POTENTIAL P(R)                                                PHF00007
C                                                                       PHF00008
C                                                                       PHF00009
      EXTERNAL P                                                        PHF00010
      REAL K1,K2,K3,K4                                                  PHF00011
    4 CONTINUE                                                          PHF00012
C                                                                       PHF00013
C   READS IN VALUES OF ENERGY IN RYDBERGS AND INCREMENT IN ATOMIC UNITS PHF00014
C                                                                       PHF00015
      READ 100,E,DR                                                     PHF00016
      IF(E .EQ. 0.0) GO TO 3                                            PHF00017
      AETA = 0.0                                                        PHF00018
      ETA = 0.0                                                         PHF00019
      R = 0.0                                                           PHF00020
C                                                                       PHF00021
C   INITIALIZE THE INTEGER COUNTER K WHICH COUNTS THE                   PHF00021
C   NUMBER OF ITERATIONS AND HENCE THE NUMBER OF INCREMENTS             PHF00021
C   DR IN THE INTEGRATION                                               PHF00021
C                                                                       PHF00021
      K = 0                                                             PHF00021
      WRITE(8,104) E                                                    PHF00022
    1 CONTINUE                                                          PHF00023
C                                                                       PHF00024
C   BEGINNING OF INTEGRATION LOOP                                       PHF00025
C                                                                       PHF00026
      AETA = ETA                                                        PHF00027
      K1 = DR*F(R,ETA,E,P)                                              PHF00028
      K2 = DR*F(R+0.5*DR,ETA+0.5*K1,E,P)                                PHF00029
      K3 = DR*F(R+0.5*DR,ETA+0.5*K2,E,P)                                PHF00030
      K4 = DR*F(R+DR,ETA+K3,E,P)                                        PHF00031
      ETA = ETA + (K1 + 2.*K2 + 2.*K3 + K4)/6.                          PHF00032
C                                                                       PHF00033
C   MODIFICATION OF EXISTING PROGRAM TO WRITE THE VALUES OF             PHF00034
C   R AND ETA IN A FILE ON DISK 8 FOR LATER RECOVERY                    PHF00035
C                                                                       PHF00036
      WRITE(8,105) R,ETA                                                PHF00037
      R = R + DR                                                        PHF00038
      K = K + 1                                                         PHF00039
C                                                                       PHF00040
C   TESTS FOR EXIT FROM INTEGRATION LOOP                                PHF00041
C                                                                       PHF00042
      TEST = ABS((ETA-AETA)/ETA)                                        PHF00043
```

```
      IF(K .LT. 1000 ) GO TO 1                                          PHF00044
      IF( TEST .LT. 1.0E-08) GO TO 2                                    PHF00045
      IF( K .GT. 18000) GO TO 2                                         PHF00046
      GO TO 1                                                           PHF00047
    2 CONTINUE                                                          PHF00048
      TNE = TAN(ETA)/E                                                  PHF00049
      PRINT 103                                                         PHF00050
      PRINT 101,E,ETA,TNE                                               PHF00051
      PRINT 102,K,TEST                                                  PHF00052
      PRINT 103                                                         PHF00053
      GO TO 4                                                           PHF00054
    3 CONTINUE                                                          PHF00055
      STOP                                                              PHF00056
  100 FORMAT(2F10.0)                                                    PHF00057
  101 FORMAT(T2,'CALOGERO PHASE SHIFT'/T5,'K = ',T9,1PE10.3/            PHF00058
     1    T5,'ETA = ',T11,1PE15.8/T5,'TANGENT(ETA)/K = ',T22,1PE15.8)   PHF00059
  102 FORMAT(//2X4HK = ,I6/2X7HTEST = ,1PE10.3)                         PHF00060
  103 FORMAT(///)                                                       PHF00061
  104 FORMAT(1H1///T2,'CALOGERO PHASE FUNCTION'/T5,'K = ',              PHF00062
     1    T9,1PE10.3//)                                                PHF00063
  105 FORMAT(5X,4HR = ,1PE13.6,5X6HETA = ,1PE13.6)                      PHF00064
      END                                                               PHF00065


      FUNCTION F(R,ETA,E,P)                                             PHF00066
C                                                                       PHF00067
C   THIS FUNCTION PROVIDES THE MAINLINE INTEGRATION ROUTINE             PHF00068
C   WITH THE FUNCTION                                                   PHF00069
C                                                                       PHF00070
C         -P(R)*SIN(KR+ETA)**2/K                                        PHF00071
C                                                                       PHF00072
C                                                                       PHF00073
      EXTERNAL P                                                        PHF00074
      F = -P(R)*SIN(E*R+ETA)**2/E                                       PHF00075
      RETURN                                                            PHF00076
      END                                                               PHF00077
```

```
      FUNCTION P(R)                                                     SCH00010
C     GAUSSIAN QUADRATURE INTEGRATION OF                                SCH00020
C     POTENTIAL FUNCTION                                                SCH00030
C                        R*INT(X**4*EXP(-R*X)DX)                        SCH00040
C                                                                       SCH00050
      SUM=0.0                                                           SCH00060
      DIMENSION A(8),X(8)                                               SCH00070
      A(1)= 0.10122854                                                  SCH00080
      A(2)= 0.22381034                                                  SCH00090
      A(3)= 0.31370665                                                  SCH00100
      A(4)= 0.36268378                                                  SCH00110
      A(5)= 0.36268378                                                  SCH00120
      A(6) = 0.31370665                                                 SCH00130
      A(7)= 0.22381034                                                  SCH00140
      A(8)= 0.10122854                                                  SCH00150
      X(1)= -0.96028986                                                 SCH00160
      X(2)= -0.79666648                                                 SCH00170
      X(3)=-0.52553241                                                  SCH00180
      X(4)= -0.18343464                                                 SCH00190
      X(5)= 0.18343464                                                  SCH00200
      X(6)= 0.52553241                                                  SCH00210
      X(7)= 0.79666648                                                  SCH00220
      X(8)= 0.96028986                                                  SCH00230
      DO 1 I = 1,8                                                      SCH00240
      U = 0.5*(X(I)+1.)                                                 SCH00250
    1 SUM = SUM + A(I)*(U**4*EXP(-R*U))                                 SCH00260
      P = R*SUM                                                         SCH00270
      RETURN                                                            SCH00280
      END                                                               SCH00290
```

```
      FUNCTION P(R)                                                     POT00010
      IF(R .EQ. 0.0) GO TO 1                                            POT00020
      G = -10.000                                                       POT00030
      M = 1.000                                                         POT00040
      P = G*EXP(-M*R)/(M*R)                                             POT00050
      RETURN                                                            POT00060
    1 CONTINUE                                                          POTCC070
      P = 0.0                                                           POT00080
      RETURN                                                            POT00090
      END                                                               POT00100
```

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13. ABSTRACT

The solutions of the phase equation for a potential with the asymptotic properties of an atomic polarization potential are studied with the intention of developing a computer program for direct integration of the phase equation for the s-wave phase shift of an arbitrary potential. Such a program is developed and its limitations are discussed. In addition, an appendix is devoted to the variational principles of Kohn and Schwinger for calculating phase shifts.

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